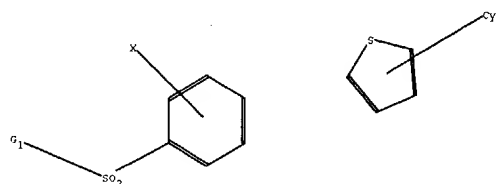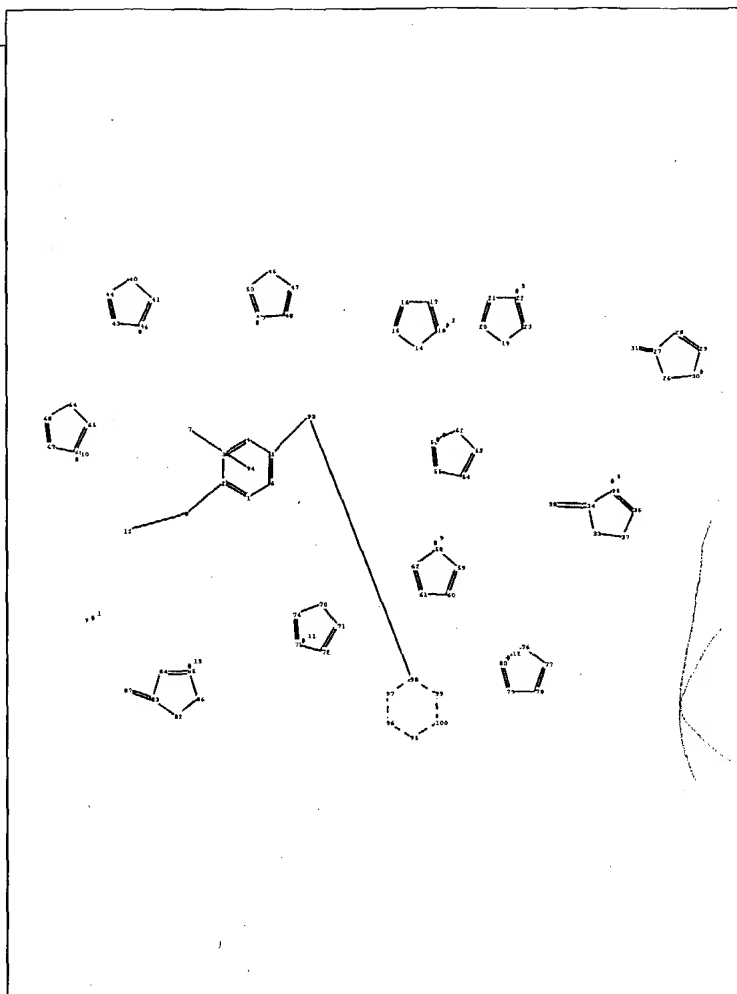chain nodes :
    7   10   16   18
ring nodes :
    1   2   3   4   5   6   11   12   13   14   15
chain bonds :
    2-7   7-10
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   11-12   11-15   12-13   13-14   14-15
exact/norm bonds :
    7-10
exact bonds :
    2-7   11-12   11-15   12-13   13-14   14-15
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
    containing 1 : 11 :

G1:Ak,NH2

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   10:CLASS   11:Atom   12:Atom
    13:Atom   14:Atom   15:Atom   16:CLASS   17:CLASS   18:Atom   19:CLASS

chain nodes :
    7   8   9   12 31 38 87 93
ring nodes :
    1   2   3   4   5   6   14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
    36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
    64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 95 96
    97 98 99 100
chain bonds :
    2-8   5-93   8-12   27-31   34-38   83-87   93-98
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21
    21-22   22-23   26-27   26-30   27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   40-41
    40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
    55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
    71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   84-85   85-86
    95-96   95-100   96-97   97-98   98-99   99-100
exact/norm bonds :
    5-93   8-12   27-31   34-38   40-41   40-44   41-42   46-47   46-50   47-48   52-53   52-56   53-54
    58-59   58-62   59-60   65-66   71-72   77-78   83-87   93-98   95-96   95-100   96-97   97-98
    98-99   99-100
exact bonds :
    2-8   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21   21-22   22-23   26-27   26-30
    27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   42-43   43-44   48-49   49-50   54-55
    55-56   60-61   61-62   64-65   64-68   66-67   67-68   70-71   70-74   72-73   73-74   76-77   76-80
    78-79   79-80   82-83   82-86   83-84   84-85   85-86
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
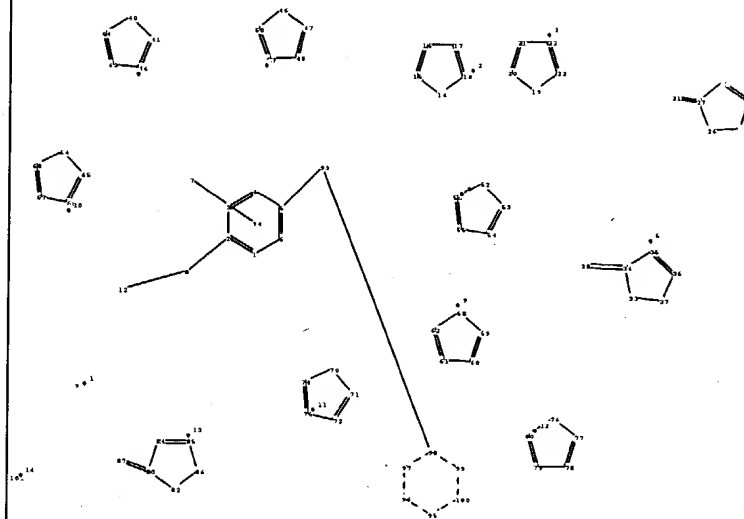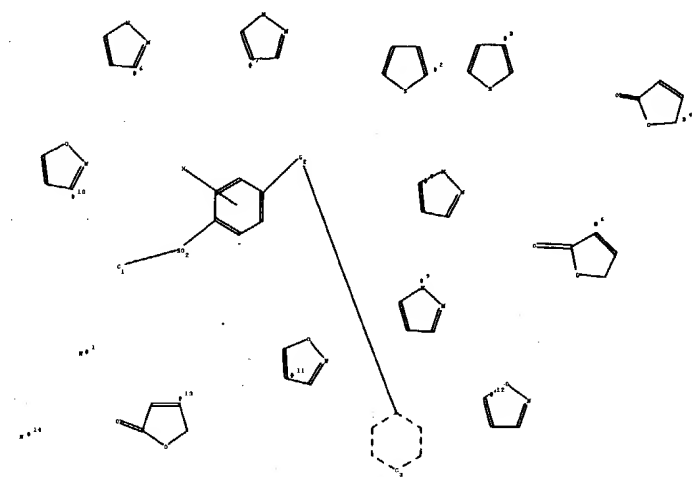   containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

```
G3:C,N

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:CLASS   12:CLASS
   14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:Atom  22:Atom  23:Atom
   26:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:CLASS  33:Atom  34:Atom  35:Atom  36:Atom
   37:Atom  38:CLASS  40:Atom  41:Atom  42:Atom  43:Atom  44:Atom  46:Atom  47:Atom  48:Atom
   49:Atom  50:Atom  52:Atom  53:Atom  54:Atom  55:Atom  56:Atom  58:Atom  59:Atom  60:Atom
   61:Atom  62:Atom  64:Atom  65:Atom  66:Atom  67:Atom  68:Atom  70:Atom  71:Atom  72:Atom
   73:Atom  74:Atom  76:Atom  77:Atom  78:Atom  79:Atom  80:Atom  82:Atom  83:Atom  84:Atom
   85:Atom  86:Atom  87:CLASS  93:CLASS  94:CLASS  95:Atom  96:Atom  97:Atom  98:Atom
   99:Atom  100:Atom
```

hain nodes :
    7   8   9   12   31   38   87   93   101
ing nodes :
    1   2   3   4   5   6   14   15   16   17   18   19   20   21   22   23   26   27   28   29   30   33   34   35
    36   37   40   41   42   43   44   46   47   48   49   50   52   53   54   55   56   58   59   60   61   62
    64   65   66   67   68   70   71   72   73   74   76   77   78   79   80   82   83   84   85   86   95   96
    97   98   99   100
hain bonds :
    2-8   5-93   8-12   27-31   34-38   83-87   93-98
ing bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21
    21-22   22-23   26-27   26-30   27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   40-41
    40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
    55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
    71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   84-85   85-86
    95-96   95-100   96-97   97-98   98-99   99-100
xact/norm bonds :
    5-93   8-12   27-31   34-38   40-41   40-44   41-42   46-47   46-50   47-48   52-53   52-56   53-54
    58-59   58-62   59-60   65-66   71-72   77-78   83-87   93-98   95-96   95-100   96-97   97-98
    98-99   99-100
xact bonds :
    2-8   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21   21-22   22-23   26-27   26-30
    27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   42-43   43-44   48-49   49-50   54-55
    55-56   60-61   61-62   64-65   64-68   66-67   67-68   70-71   70-74   72-73   73-74   76-77   76-80
    78-79   79-80   82-83   82-86   83-84   84-85   85-86
ormalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
olated ring systems :
    containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :
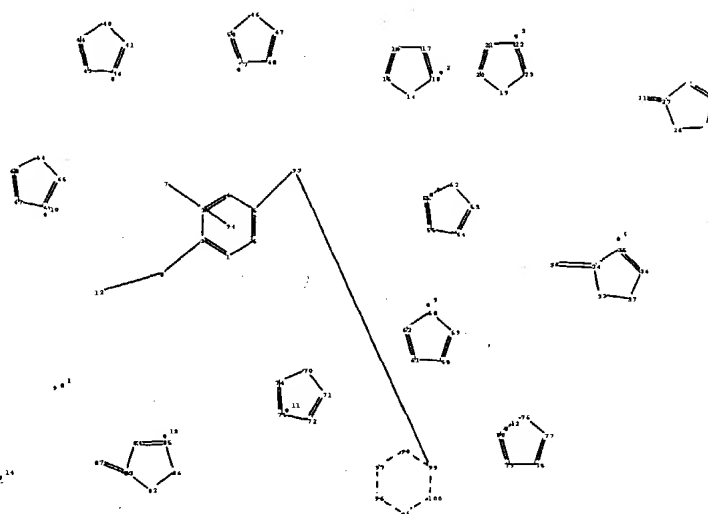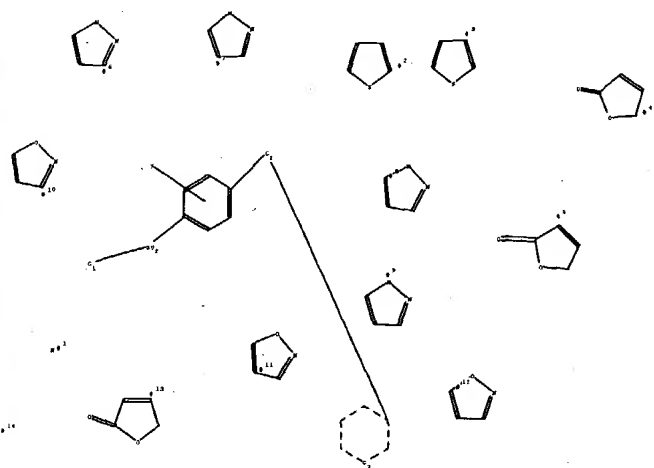
:CH3,Et,[*1]

:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

```
G3:C,[*14]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:CLASS   12:CLASS
   14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:Atom  22:Atom  23:Atom
   26:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:CLASS  33:Atom  34:Atom  35:Atom  36:Atom
   37:Atom  38:CLASS  40:Atom  41:Atom  42:Atom  43:Atom  44:Atom  46:Atom  47:Atom  48:Atom
   49:Atom  50:Atom  52:Atom  53:Atom  54:Atom  55:Atom  56:Atom  58:Atom  59:Atom  60:Atom
   61:Atom  62:Atom  64:Atom  65:Atom  66:Atom  67:Atom  68:Atom  70:Atom  71:Atom  72:Atom
   73:Atom  74:Atom  76:Atom  77:Atom  78:Atom  79:Atom  80:Atom  82:Atom  83:Atom  84:Atom
   85:Atom  86:Atom  87:CLASS  93:CLASS  94:CLASS  95:Atom  96:Atom  97:Atom  98:Atom
   99:Atom  100:Atom  101:CLASS
```

C:\stnweb\Queries\1.str

chain nodes :
      7   8   9   12 31 38 87 93 101
ring nodes :
      1   2   3   4   5   6   14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
      36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
      64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 95 96
      97 98 99 100
chain bonds :
      2-8   5-93   8-12   27-31   34-38   83-87   93-99
ring bonds :
      1-2   1-6   2-3   3-4   4-5   5-6   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21
      21-22   22-23   26-27   26-30   27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   40-41
      40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
      55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
      71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   84-85   85-86
      95-96   95-100   96-97   97-98   98-99   99-100
exact/norm bonds :
      5-93   8-12   27-31   34-38   40-41   40-44   41-42   46-47   46-50   47-48   52-53   52-56   53-54
      58-59   58-62   59-60   65-66   71-72   77-78   83-87   93-99   95-96   95-100   96-97   97-98
      98-99   99-100
exact bonds :
      2-8   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21   21-22   22-23   26-27   26-30
      27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   42-43   43-44   48-49   49-50   54-55
      55-56   60-61   61-62   64-65   64-68   66-67   67-68   70-71   70-74   72-73   73-74   76-77   76-80
      78-79   79-80   82-83   82-86   83-84   84-85   85-86
normalized bonds :
      1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
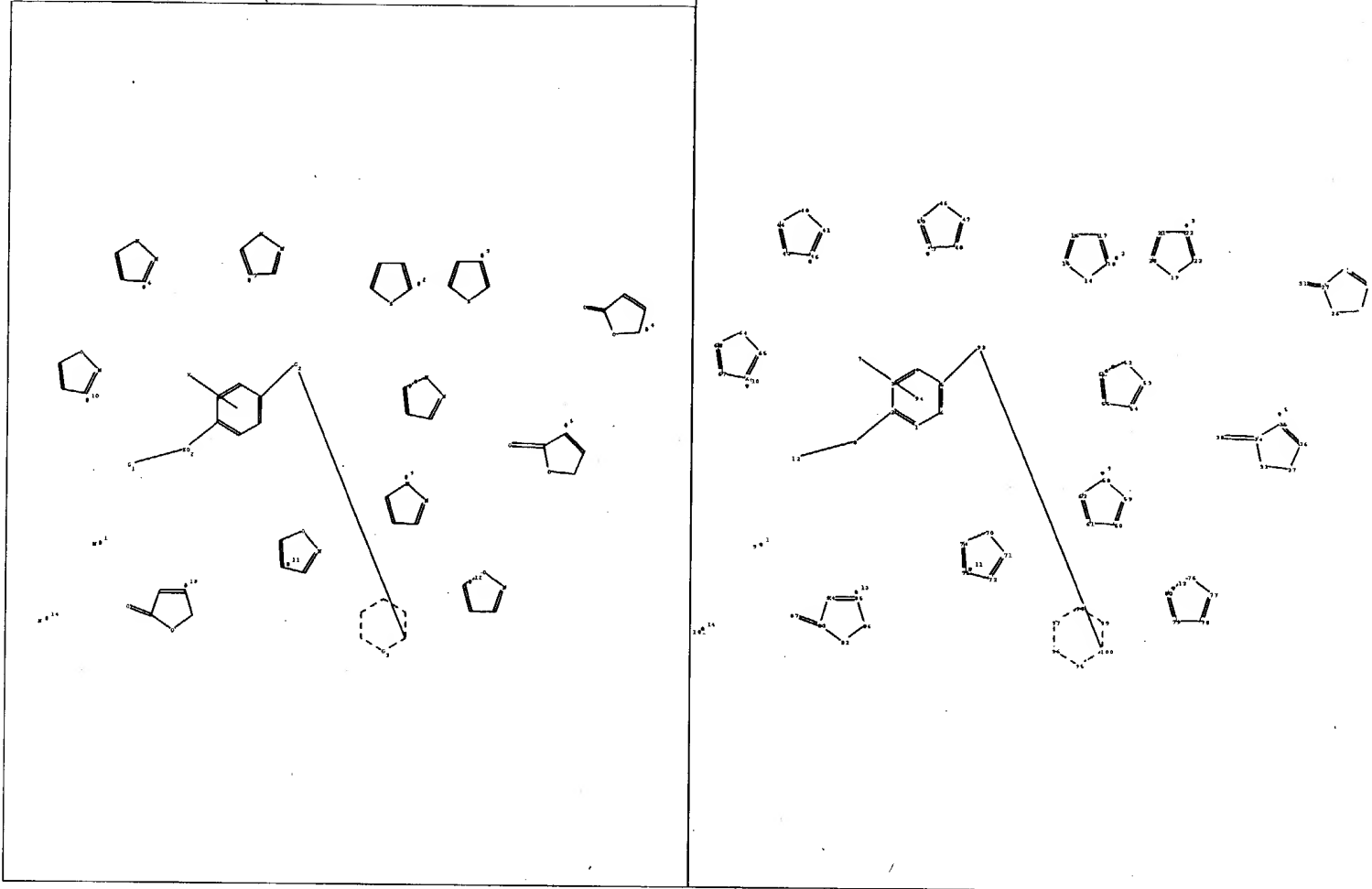   containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

1:CH3,Et,[*1]

2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,[*14]

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
    14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
    26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
    37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
    49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
    61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
    73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
    85:Atom 86:Atom 87:CLASS 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom
    99:Atom 100:Atom 101:CLASS

chain nodes :
    7   8   9   12   31   38   87   93   101
ring nodes :
    1   2   3   4   5   6   14   15   16   17   18   19   20   21   22   23   26   27   28   29   30   33   34   35
    36   37   40   41   42   43   44   46   47   48   49   50   52   53   54   55   56   58   59   60   61   62
    64   65   66   67   68   70   71   72   73   74   76   77   78   79   80   82   83   84   85   86   95   96
    97   98   99   100
chain bonds :
    2-8   5-93   8-12   27-31   34-38   83-87   93-100
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21
    21-22   22-23   26-27   26-30   27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   40-41
    40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
    55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
    71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   84-85   85-86
    95-96   95-100   96-97   97-98   98-99   99-100
exact/norm bonds :
    5-93   8-12   27-31   34-38   40-41   40-44   41-42   46-47   46-50   47-48   52-53   52-56   53-54
    58-59   58-62   59-60   65-66   71-72   77-78   83-87   93-100   95-96   95-100   96-97   97-98
    98-99   99-100
exact bonds :
    2-8   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21   21-22   22-23   26-27   26-30
    27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   42-43   43-44   48-49   49-50   54-55
    55-56   60-61   61-62   64-65   64-68   66-67   67-68   70-71   70-74   72-73   73-74   76-77   76-80
    78-79   79-80   82-83   82-86   83-84   84-85   85-86
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
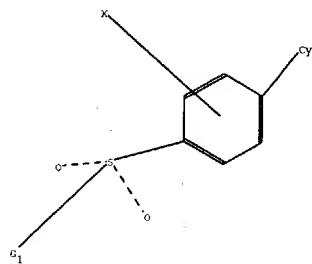   containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]
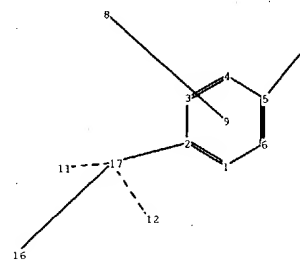
c,[*14]

ch level :
```
 1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:CLASS  12:CLASS
14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:Atom  22:Atom  23:Atom
26:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:CLASS  33:Atom  34:Atom  35:Atom  36:Atom
37:Atom  38:CLASS  40:Atom  41:Atom  42:Atom  43:Atom  44:Atom  46:Atom  47:Atom  48:Atom
49:Atom  50:Atom  52:Atom  53:Atom  54:Atom  55:Atom  56:Atom  58:Atom  59:Atom  60:Atom
61:Atom  62:Atom  64:Atom  65:Atom  66:Atom  67:Atom  68:Atom  70:Atom  71:Atom  72:Atom
73:Atom  74:Atom  76:Atom  77:Atom  78:Atom  79:Atom  80:Atom  82:Atom  83:Atom  84:Atom
85:Atom  86:Atom  87:CLASS  93:CLASS  94:CLASS  95:Atom  96:Atom  97:Atom  98:Atom
99:Atom  100:Atom  101:CLASS
```
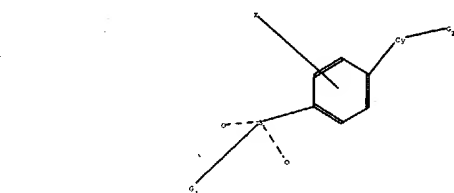
chain nodes :
    7   8   11   12   13   16   17
ring nodes :
    1   2   3   4   5   6
chain bonds :
    2-17   5-7   11-17   12-17   16-17
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
exact/norm bonds :
    2-17   5-7   11-17   12-17   16-17
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
    containing 1 :

G1:CH3,Et,[*1]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:CLASS   9:CLASS   11:CLASS
    12:CLASS   13:CLASS   16:CLASS   17:CLASS
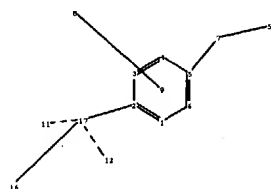
chain nodes :
    7   8   11   12   13   16   17   54
ring nodes :
    1   2   3   4   5   6   18   19   20   21   22   23   24   25   26   27   28   29   30   31   32   33   34   35
    36   37   38   39   40   41   42   43   44   45   46   47
chain bonds :
    2-17   5-7   7-54   11-17   12-17   16-17
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   18-19   18-23   19-20   20-21   21-22   22-23   24-25   24-29
    25-26   26-27   27-28   28-29   30-31   30-35   31-32   32-33   33-34   34-35   .36-37   36-41   37-38
    38-39   39-40   40-41   42-43   42-47   43-44   44-45   45-46   46-47
exact/norm bonds :
    2-17   5-7   7-54   11-17   12-17   16-17
exact bonds :
    18-19   18-23   19-20   20-21   21-22   22-23
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   24-25   24-29   25-26   26-27   27-28   28-29   30-31   30-35
    31-32   32-33   33-34   34-35   36-37   36-41   37-38   38-39   39-40   40-41   42-43   42-47   43-44
    44-45   45-46   46-47
isolated ring systems :
    containing 1 : 18 : 24 : 30 : 36 : 42 :

G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:CLASS   9:CLASS   11:CLASS
    12:CLASS   13:CLASS   16:CLASS   17:CLASS   18:Atom   19:Atom   20:Atom   21:Atom   22:Atom
    23:Atom   24:Atom   25:Atom   26:Atom   27:Atom   28:Atom   29:Atom   30:Atom   31:Atom   32:Atom
    33:Atom   34:Atom   35:Atom   36:Atom   37:Atom   38:Atom   39:Atom   40:Atom   41:Atom   42:Atom
    43:Atom   44:Atom   45:Atom   46:Atom   47:Atom   54:CLASS
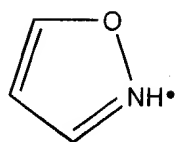
isoxazolyl
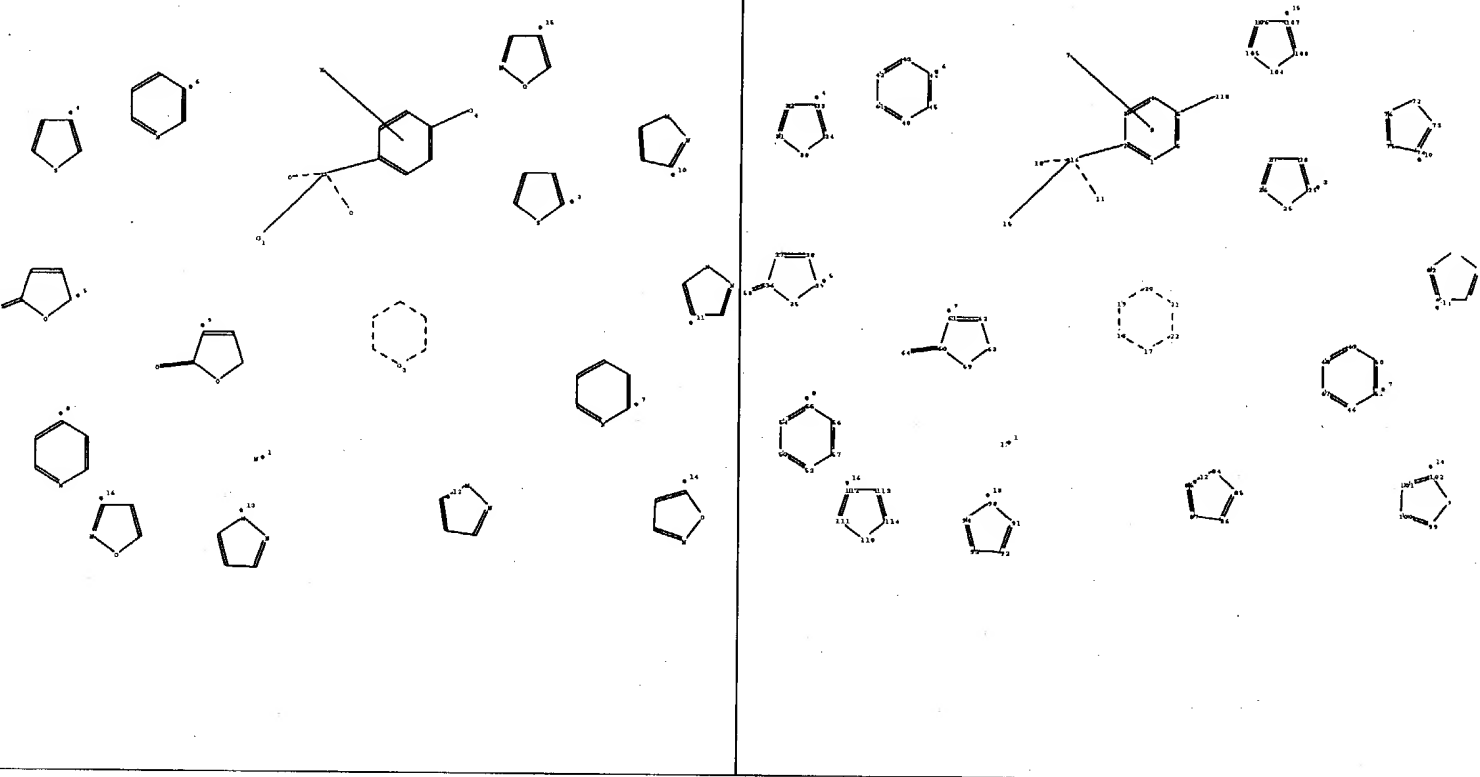
chain nodes :
      7   10   11   12   15   16   58   64   118
ring nodes :
      1   2   3   4   5   6   17   18   19   20   21   22   25   26   27   28   29   30   31   32   33   34   35   36
     37   38   39   40   41   42   43   44   45   46   47   48   49   50   51   52   53   54   55   56   57   59
     60   61   62   63   72   73   74   75   76   78   79   80   81   82   84   85   86   87   88   90   91   92
     93   94   98   99 100 101 102 104 105 106 107 108 110 111 112 113 114
chain bonds :
     2-16   5-118   10-16   11-16   15-16   36-58   60-64
ring bonds :
     1-2   1-6   2-3   3-4   4-5   5-6   17-18   17-22   18-19   19-20   20-21   21-22   25-26   25-29
     26-27   27-28   28-29   30-31   30-34   31-32   32-33   33-34   35-36   35-39   36-37   37-38   38-39
     40-41   40-45   41-42   42-43   43-44   44-45   46-47   46-51   47-48   48-49   49-50   50-51   52-53
     52-57   53-54   54-55   55-56   56-57   59-60   59-63   60-61   61-62   62-63   72-73   72-76   73-74
     74-75   75-76   78-79   78-82   79-80   80-81   81-82   84-85   84-88   85-86   86-87   87-88   90-91
     90-94   91-92   92-93   93-94   98-99   98-102   99-100   100-101   101-102   104-105   104-108
    105-106   106-107   107-108   110-111   110-114   111-112   112-113   113-114
exact/norm bonds :
     2-16   5-118   10-16   11-16   15-16   17-18   17-22   18-19   19-20   20-21   21-22   25-26   25-29
     26-27   27-28   28-29   30-31   30-34   31-32   32-33   33-34   35-36   35-39   36-37   36-58   37-38
     38-39   59-60   59-63   60-61   60-64   61-62   62-63   72-73   72-76   73-74   74-75   75-76   78-79
     78-82   79-80   80-81   81-82   84-85   84-88   85-86   86-87   87-88   90-91   90-94   91-92   92-93
     93-94   98-99   98-102   99-100   100-101   101-102   104-105   104-108   105-106   106-107
    107-108   110-111   110-114   111-112   112-113   113-114
normalized bonds :
     1-2   1-6   2-3   3-4   4-5   5-6   40-41   40-45   41-42   42-43   43-44   44-45   46-47   46-51
     47-48   48-49   49-50   50-51   52-53   52-57   53-54   54-55   55-56   56-57
isolated ring systems :
      containing 1 : 17 : 25 : 30 : 35 : 40 : 46 : 52 : 59 : 72 : 78 : 84 : 90 : 110 :

1:CH3,Et,[*1]

2

G3:C,N

G4:[*1],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15],[*16]

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS
    12:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
    25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom
    35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom
    45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:CLASS
    54:CLASS 55:Atom 56:Atom 57:Atom 58:CLASS 59:Atom 60:Atom 61:Atom 62:Atom
    63:Atom 64:CLASS 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 78:Atom 79:Atom 80:Atom
    81:Atom 82:Atom 84:Atom 85:Atom 86:Atom 87:Atom 88:Atom 90:Atom 91:Atom 92:Atom
    93:Atom 94:Atom 98:Atom 99:Atom 100:Atom 101:Atom 102:Atom 104:Atom 105:Atom
    106:Atom 107:Atom 108:Atom 110:Atom 111:Atom 112:Atom 113:Atom 114:Atom 118:CLASS
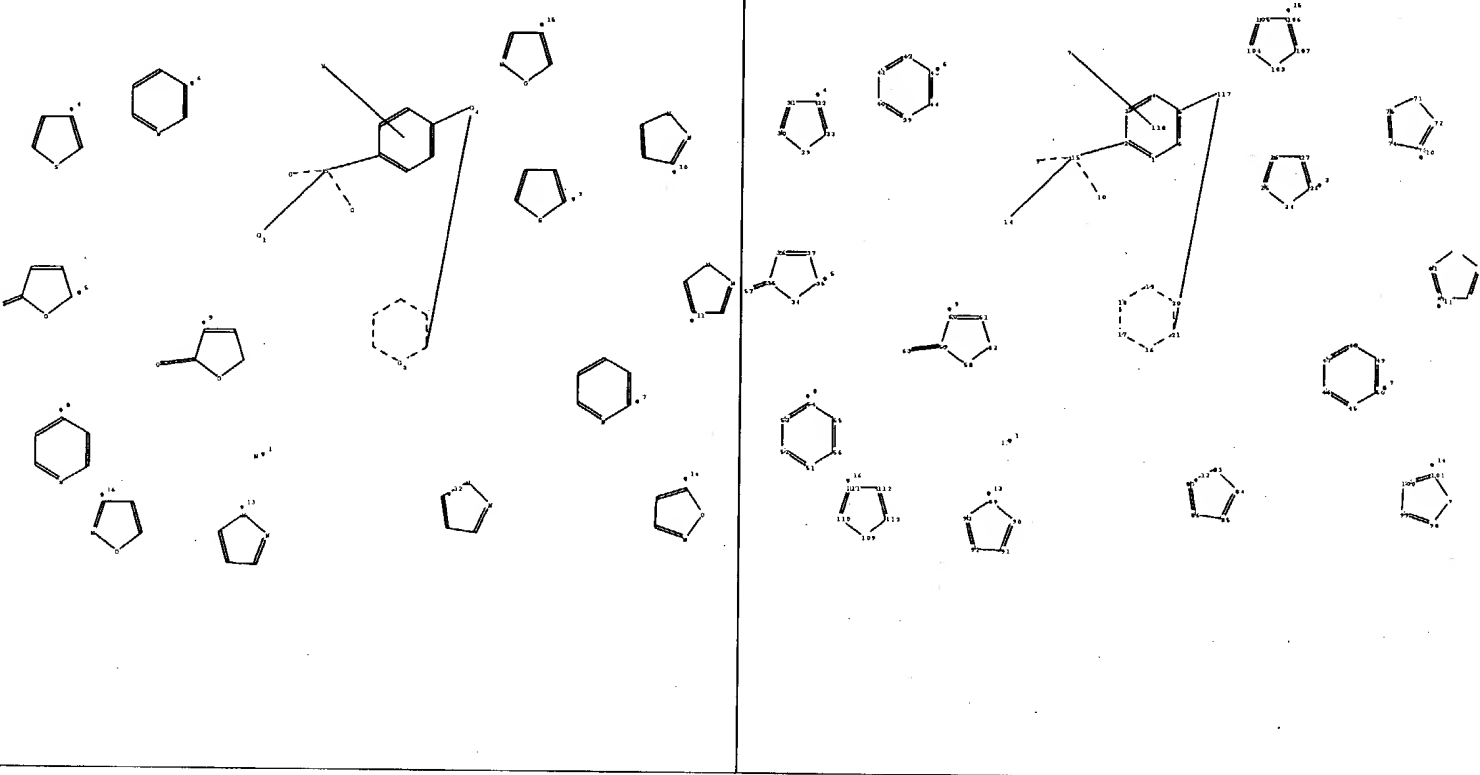
chain nodes :
    7   9   10   11   14   15   57   63   117
ring nodes :
    1   2   3   4   5   6   16   17   18   19   20   21   24   25   26   27   28   29   30   31   32   33   34   35
    36   37   38   39   40   41   42   43   44   45   46   47   48   49   50   51   52   53   54   55   56   58
    59   60   61   62   71   72   73   74   75   77   78   79   80   81   83   84   85   86   87   89   90   91
    92   93   97   98   99   100   101   103   104   105   106   107   109   110   111   112   113
chain bonds :
    2-15   5-117   9-15   10-15   14-15   21-117   35-57   59-63
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   16-17   16-21   17-18   18-19   19-20   20-21   24-25   24-28
    25-26   26-27   27-28   29-30   29-33   30-31   31-32   32-33   34-35   34-38   35-36   36-37   37-38
    39-40   39-44   40-41   41-42   42-43   43-44   45-46   45-50   46-47   47-48   48-49   49-50   51-52
    51-56   52-53   53-54   54-55   55-56   58-59   58-62   59-60   60-61   61-62   71-72   71-75   72-73
    73-74   74-75   77-78   77-81   78-79   79-80   80-81   83-84   83-87   84-85   85-86   86-87   89-90
    89-93   90-91   91-92   92-93   97-98   97-101   98-99   99-100   100-101   103-104   103-107
    104-105   105-106   106-107   109-110   109-113   110-111   111-112   112-113
exact/norm bonds :
    2-15   5-117   9-15   10-15   14-15   16-17   16-21   17-18   18-19   19-20   20-21   21-117   24-25
    24-28   25-26   26-27   27-28   29-30   29-33   30-31   31-32   32-33   34-35   34-38   35-36   35-57
    36-37   37-38   58-59   58-62   59-60   59-63   60-61   61-62   71-72   71-75   72-73   73-74   74-75
    77-78   77-81   78-79   79-80   80-81   83-84   83-87   84-85   85-86   86-87   89-90   89-93   90-91
    91-92   92-93   97-98   97-101   98-99   99-100   100-101   103-104   103-107   104-105   105-106
    106-107   109-110   109-113   110-111   111-112   112-113
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   39-40   39-44   40-41   41-42   42-43   43-44   45-46   45-50
    46-47   47-48   48-49   49-50   51-52   51-56   52-53   53-54   54-55   55-56
isolated ring systems :
   containing 1 : 16 : 24 : 29 : 34 : 39 : 45 : 51 : 58 : 71 : 77 : 83 : 89 : 109 :

1:CH3,Et,[*1]

2

G3:C,N

G4:[*1],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15],[*16]

Match level :
```
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   9:CLASS   10:CLASS   11:CLASS
    14:CLASS  15:CLASS  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:Atom  24:Atom
    25:Atom  26:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:Atom  32:Atom  33:Atom  34:Atom
    35:Atom  36:Atom  37:Atom  38:Atom  39:Atom  40:Atom  41:Atom  42:Atom  43:Atom  44:Atom
    45:Atom  46:Atom  47:Atom  48:Atom  49:Atom  50:Atom  51:Atom  52:Atom  53:Atom  54:Atom
    55:Atom  56:Atom  57:CLASS  58:Atom  59:Atom  60:Atom  61:Atom  62:Atom  63:CLASS
    71:Atom  72:Atom  73:Atom  74:Atom  75:Atom  77:Atom  78:Atom  79:Atom  80:Atom  81:Atom
    83:Atom  84:Atom  85:Atom  86:Atom  87:Atom  89:Atom  90:Atom  91:Atom  92:Atom  93:Atom
    97:Atom  98:Atom  99:Atom  100:Atom  101:Atom  103:Atom  104:Atom  105:Atom  106:Atom
    107:Atom  109:Atom  110:Atom  111:Atom  112:Atom  113:Atom  117:CLASS  118:CLASS
```
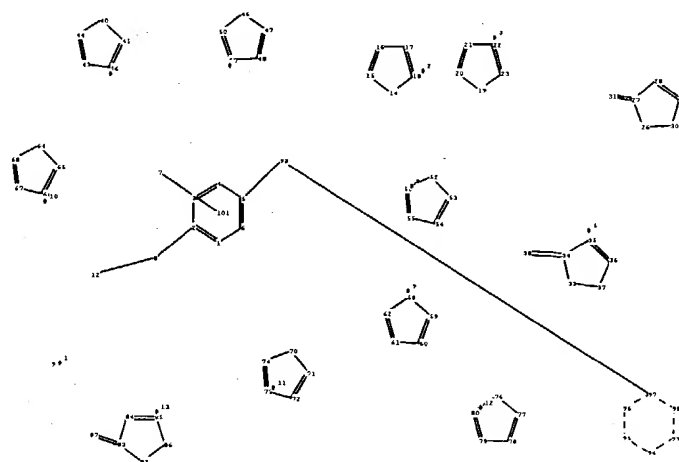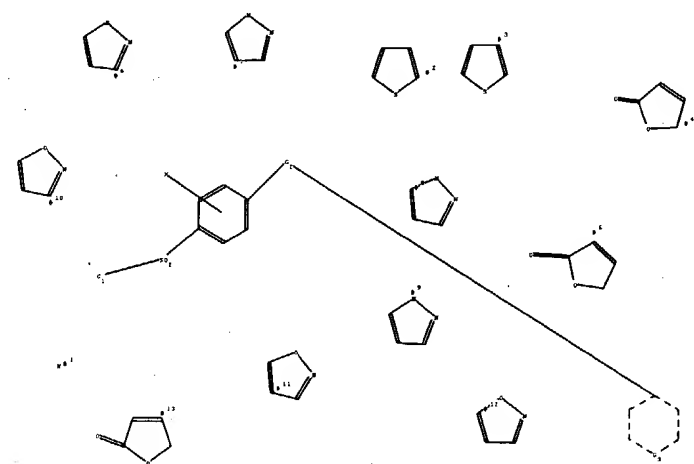
nain nodes :
    7   8   9   12 31 38 87 93
ing nodes :
    1   2   3   4   5   6   14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
    36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
    64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 94 95
    96 97 98 99
nain bonds :
    2-8   5-93 8-12 27-31 34-38 83-87 93-97
ng bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21
    21-22 22-23 26-27 26-30 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 40-41
    40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
    55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
    71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 84-85 85-86
    94-95 94-99 95-96 96-97 97-98 98-99
act/norm bonds :
    2-8   5-93 8-12 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23
    26-27 26-30 27-28 27-31 28-29 29-30 33-34 33-37 34-35 34-38 35-36 36-37 40-41
    40-44 41-42 42-43 43-44 46-47 46-50 47-48 48-49 49-50 52-53 52-56 53-54 54-55
    55-56 58-59 58-62 59-60 60-61 61-62 64-65 64-68 65-66 66-67 67-68 70-71 70-74
    71-72 72-73 73-74 76-77 76-80 77-78 78-79 79-80 82-83 82-86 83-84 83-87 84-85
    85-86 93-97 94-95 94-99 95-96 96-97 97-98 98-99
rmalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
olated ring systems :
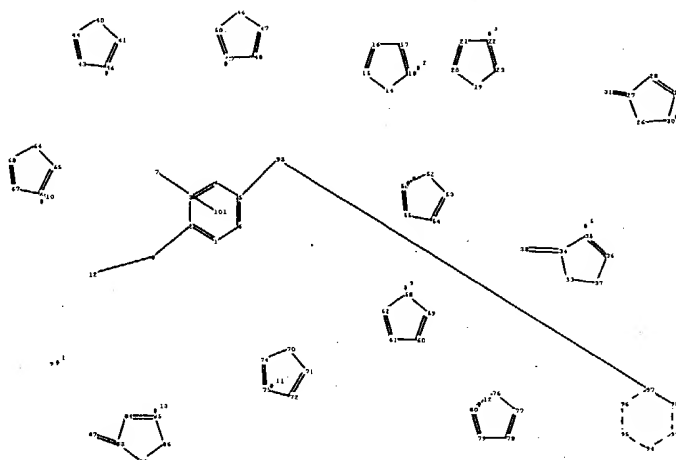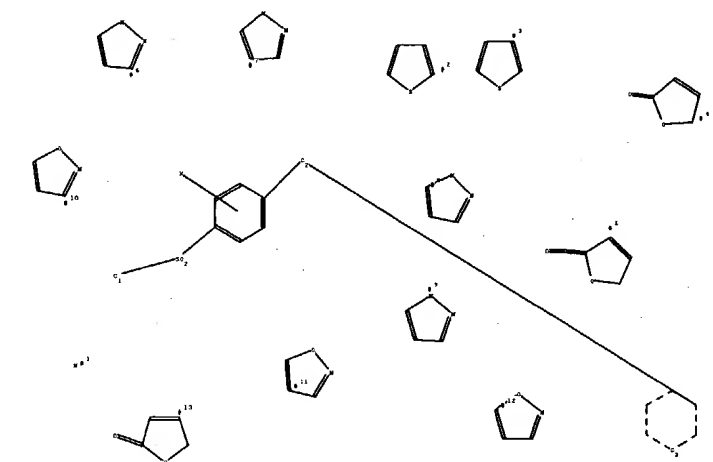   containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

:CH3,Et,[*1]

:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

:C,N

```
Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:CLASS   12:CLASS
   14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom   21:Atom   22:Atom   23:Atom
   26:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:CLASS  33:Atom   34:Atom   35:Atom   36:Atom
   37:Atom  38:CLASS  40:Atom  41:Atom  42:Atom  43:Atom  44:Atom   46:Atom   47:Atom   48:Atom
   49:Atom  50:Atom  52:Atom  53:Atom  54:Atom  55:Atom  56:Atom   58:Atom   59:Atom   60:Atom
   61:Atom  62:Atom  64:Atom  65:Atom  66:Atom  67:Atom  68:Atom   70:Atom   71:Atom   72:Atom
   73:Atom  74:Atom  76:Atom  77:Atom  78:Atom  79:Atom  80:Atom   82:Atom   83:Atom   84:Atom
   85:Atom  86:Atom  87:CLASS  93:CLASS  94:Atom  95:Atom  96:Atom   97:Atom   98:Atom
   99:Atom  101:CLASS
```

C:\stnweb\Queries\5b.str

chain nodes :
    7   8   9   12 31 38 87 93
ring nodes :
    1   2   3   4   5   6   14 15 16 17 18 19 20 21 22 23 26 27 28 29 30 33 34 35
    36 37 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56 58 59 60 61 62
    64 65 66 67 68 70 71 72 73 74 76 77 78 79 80 82 83 84 85 86 94 95
    96 97 98 99
chain bonds :
    2-8   5-93   8-12   27-31   34-38   83-87   93-98
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21
    21-22   22-23   26-27   26-30   27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   40-41
    40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
    55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
    71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   84-85   85-86
    94-95   94-99   95-96   96-97   97-98   98-99
exact/norm bonds :
    2-8   5-93   8-12   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21   21-22   22-23
    26-27   26-30   27-28   27-31   28-29   29-30   33-34   33-37   34-35   34-38   35-36   36-37   40-41
    40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
    55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
    71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   83-87   84-85
    85-86   93-98   94-95   94-99   95-96   96-97   97-98   98-99
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
    containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :
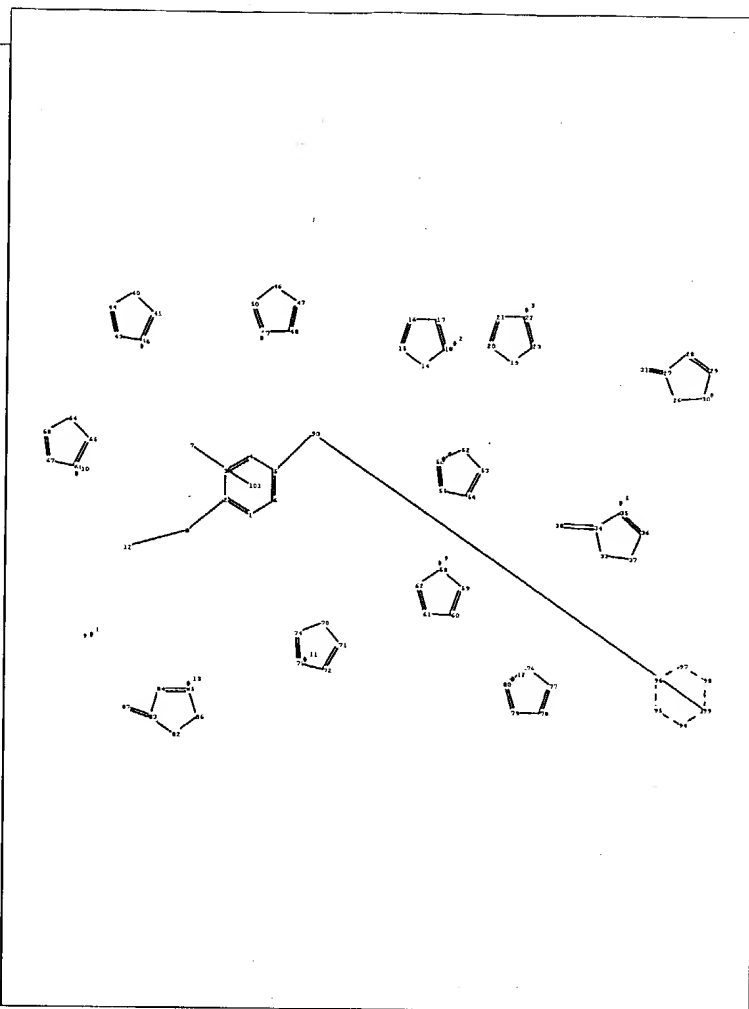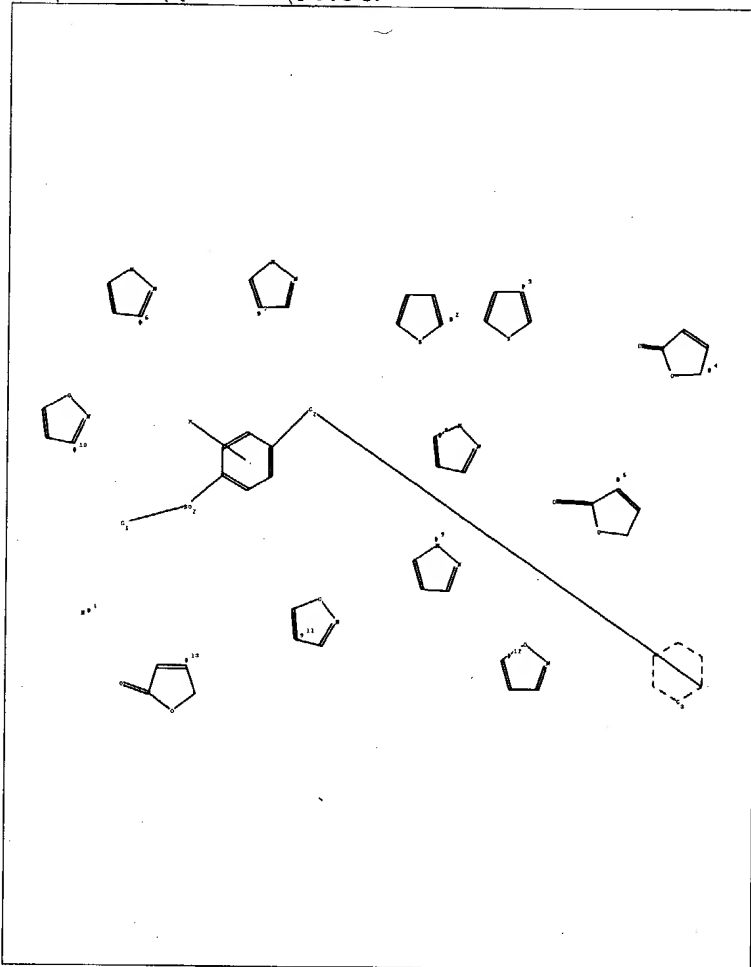
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

Match level :
     1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:CLASS   12:CLASS
     14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:Atom   21:Atom   22:Atom   23:Atom
     26:Atom   27:Atom   28:Atom   29:Atom   30:Atom   31:CLASS   33:Atom   34:Atom   35:Atom   36:Atom
     37:Atom   38:CLASS   40:Atom   41:Atom   42:Atom   43:Atom   44:Atom   46:Atom   47:Atom   48:Atom
     49:Atom   50:Atom   52:Atom   53:Atom   54:Atom   55:Atom   56:Atom   58:Atom   59:Atom   60:Atom
     61:Atom   62:Atom   64:Atom   65:Atom   66:Atom   67:Atom   68:Atom   70:Atom   71:Atom   72:Atom
     73:Atom   74:Atom   76:Atom   77:Atom   78:Atom   79:Atom   80:Atom   82:Atom   83:Atom   84:Atom
     85:Atom   86:Atom   87:CLASS   93:CLASS   94:Atom   95:Atom   96:Atom   97:Atom   98:Atom
     99:Atom   101:CLASS

chain nodes :
    7   8   9   12   31   38   87   93
ring nodes :
    1   2   3   4   5   6   14   15   16   17   18   19   20   21   22   23   26   27   28   29   30   33   34   35
    36   37   40   41   42   43   44   46   47   48   49   50   52   53   54   55   56   58   59   60   61   62
    64   65   66   67   68   70   71   72   73   74   76   77   78   79   80   82   83   84   85   86   94   95
    96   97   98   99
chain bonds :
    2-8   5-93   8-12   27-31   34-38   83-87   93-99
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21
    21-22   22-23   26-27   26-30   27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   40-41
    40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
    55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
    71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   84-85   85-86
    94-95   94-99   95-96   96-97   97-98   98-99
exact/norm bonds :
    2-8   5-93   8-12   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21   21-22   22-23
    26-27   26-30   27-28   27-31   28-29   29-30   33-34   33-37   34-35   34-38   35-36   36-37   40-41
    40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
    55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
    71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   83-87   84-85
    85-86   93-99   94-95   94-99   95-96   96-97   97-98   98-99
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
    containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]
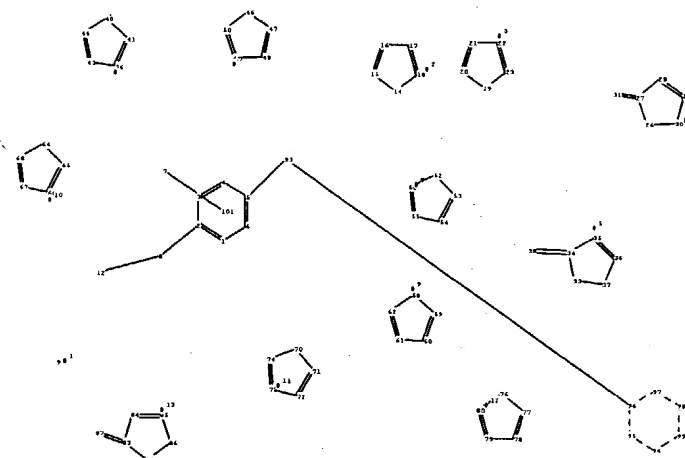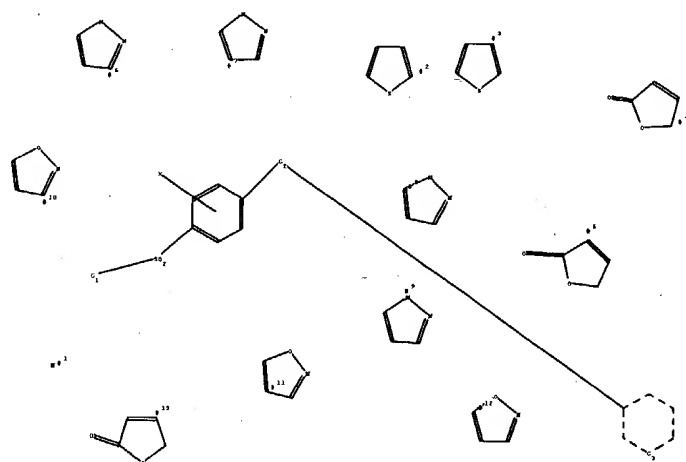
G3:C,N

atch level :
```
 1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:CLASS   12:CLASS
14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:Atom  22:Atom  23:Atom
26:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:CLASS  33:Atom  34:Atom  35:Atom  36:Atom
37:Atom  38:CLASS  40:Atom  41:Atom  42:Atom  43:Atom  44:Atom  46:Atom  47:Atom  48:Atom
49:Atom  50:Atom  52:Atom  53:Atom  54:Atom  55:Atom  56:Atom  58:Atom  59:Atom  60:Atom
61:Atom  62:Atom  64:Atom  65:Atom  66:Atom  67:Atom  68:Atom  70:Atom  71:Atom  72:Atom
73:Atom  74:Atom  76:Atom  77:Atom  78:Atom  79:Atom  80:Atom  82:Atom  83:Atom  84:Atom
85:Atom  86:Atom  87:CLASS  93:CLASS  94:Atom  95:Atom  96:Atom  97:Atom  98:Atom
99:Atom  101:CLASS
```

```
chain nodes :
    7   8   9  12  31  38  87  93
ring nodes :
    1   2   3   4   5   6  14  15  16  17  18  19  20  21  22  23  26  27  28  29  30  33  34  35
   36  37  40  41  42  43  44  46  47  48  49  50  52  53  54  55  56  58  59  60  61  62
   64  65  66  67  68  70  71  72  73  74  76  77  78  79  80  82  83  84  85  86  94  95
   96  97  98  99
chain bonds :
    2-8   5-93   8-12   27-31   34-38   83-87   93-96
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21
   21-22   22-23   26-27   26-30   27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   40-41
   40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
   55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
   71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   84-85   85-86
   94-95   94-99   95-96   96-97   97-98   98-99
exact/norm bonds :
    2-8   5-93   8-12   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21   21-22   22-23
   26-27   26-30   27-28   27-31   28-29   29-30   33-34   33-37   34-35   34-38   35-36   36-37   40-41
   40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
   55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
   71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   83-87   84-85
   85-86   93-96   94-95   94-99   95-96   96-97   97-98   98-99
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
    containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :
```
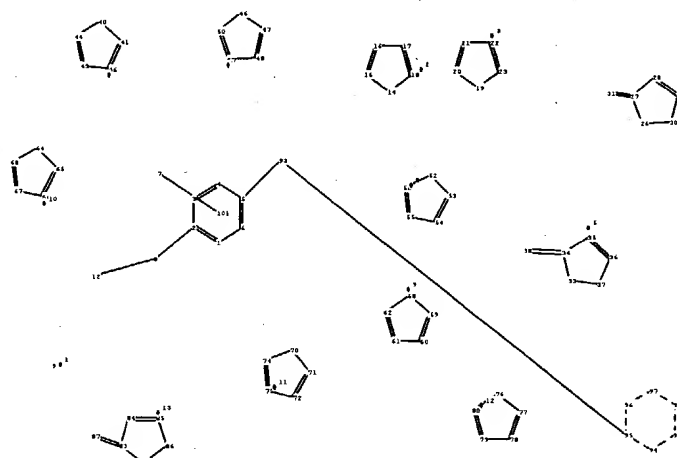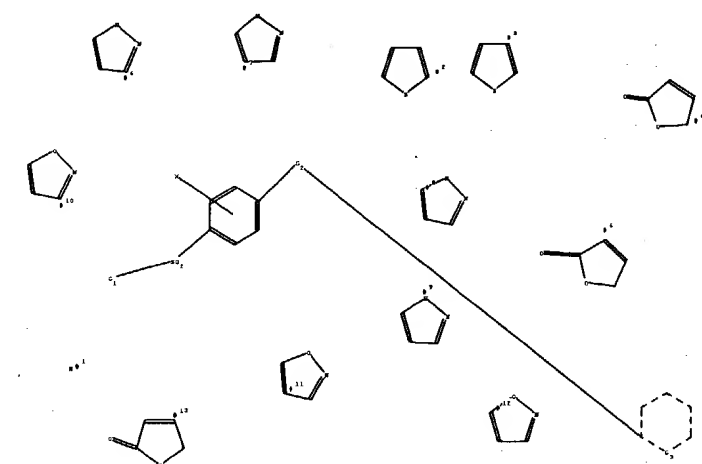
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

```
Match level :
  1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:CLASS   12:CLASS
  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom   21:Atom   22:Atom   23:Atom
  26:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:CLASS  33:Atom   34:Atom   35:Atom   36:Atom
  37:Atom  38:CLASS  40:Atom  41:Atom  42:Atom  43:Atom  44:Atom   46:Atom   47:Atom   48:Atom
  49:Atom  50:Atom  52:Atom  53:Atom  54:Atom  55:Atom  56:Atom   58:Atom   59:Atom   60:Atom
  61:Atom  62:Atom  64:Atom  65:Atom  66:Atom  67:Atom  68:Atom   70:Atom   71:Atom   72:Atom
  73:Atom  74:Atom  76:Atom  77:Atom  78:Atom  79:Atom  80:Atom   82:Atom   83:Atom   84:Atom
  85:Atom  86:Atom  87:CLASS  93:CLASS  94:Atom  95:Atom  96:Atom  97:Atom  98:Atom
  99:Atom  101:CLASS
```

```
chain nodes :
     7   8   9   12   31   38   87   93
ring nodes :
     1    2    3    4    5    6   14   15   16   17   18   19   20   21   22   23   26   27   28   29   30   33   34   35
    36   37   40   41   42   43   44   46   47   48   49   50   52   53   54   55   56   58   59   60   61   62
    64   65   66   67   68   70   71   72   73   74   76   77   78   79   80   82   83   84   85   86   94   95
    96   97   98   99
chain bonds :
     2-8   5-93   8-12   27-31   34-38   83-87   93-95
ring bonds :
     1-2    1-6    2-3    3-4    4-5    5-6   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21
    21-22   22-23   26-27   26-30   27-28   28-29   29-30   33-34   33-37   34-35   35-36   36-37   40-41
    40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
    55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
    71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   84-85   85-86
    94-95   94-99   95-96   96-97   97-98   98-99
exact/norm bonds :
     2-8   5-93   8-12   14-15   14-18   15-16   16-17   17-18   19-20   19-23   20-21   21-22   22-23
    26-27   26-30   27-28   27-31   28-29   29-30   33-34   33-37   34-35   34-38   35-36   36-37   40-41
    40-44   41-42   42-43   43-44   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
    55-56   58-59   58-62   59-60   60-61   61-62   64-65   64-68   65-66   66-67   67-68   70-71   70-74
    71-72   72-73   73-74   76-77   76-80   77-78   78-79   79-80   82-83   82-86   83-84   83-87   84-85
    85-86   93-95   94-95   94-99   95-96   96-97   97-98   98-99
normalized bonds :
     1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
     containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N
```
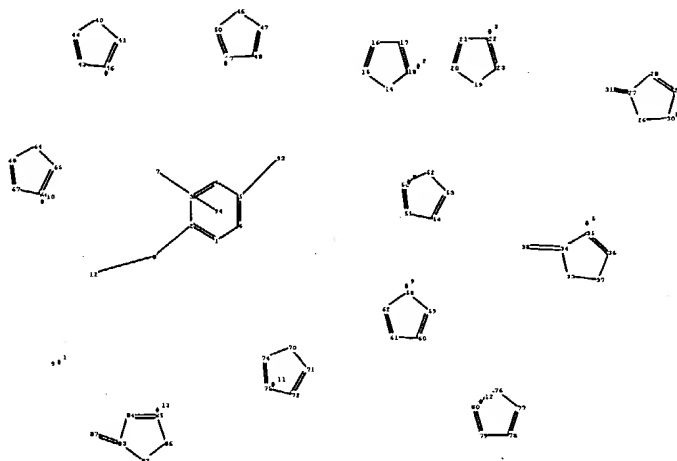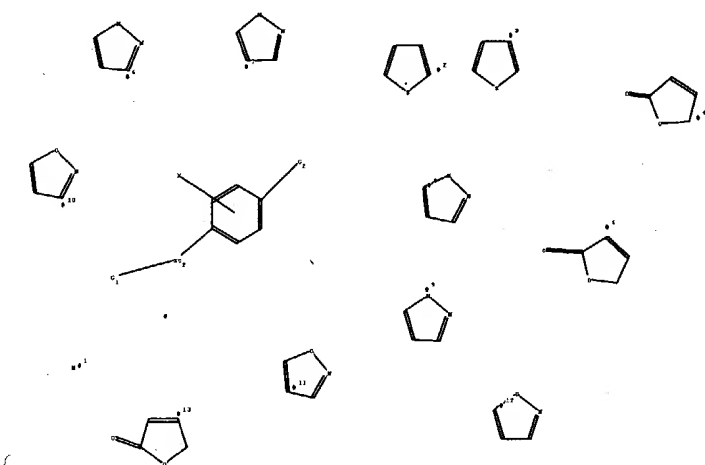
```
Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:CLASS   12:CLASS
   14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:Atom  22:Atom  23:Atom
   26:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:CLASS  33:Atom  34:Atom  35:Atom  36:Atom
   37:Atom  38:CLASS  40:Atom  41:Atom  42:Atom  43:Atom  44:Atom  46:Atom  47:Atom  48:Atom
   49:Atom  50:Atom  52:Atom  53:Atom  54:Atom  55:Atom  56:Atom  58:Atom  59:Atom  60:Atom
   61:Atom  62:Atom  64:Atom  65:Atom  66:Atom  67:Atom  68:Atom  70:Atom  71:Atom  72:Atom
   73:Atom  74:Atom  76:Atom  77:Atom  78:Atom  79:Atom  80:Atom  82:Atom  83:Atom  84:Atom
   85:Atom  86:Atom  87:CLASS  93:CLASS  94:Atom  95:Atom  96:Atom  97:Atom  98:Atom
   99:Atom  101:CLASS
```

```
chain nodes :
    7   8   9   12  31  38  87  93
ring nodes :
    1   2   3   4   5   6   14  15  16  17  18  19  20  21  22  23  26  27  28  29  30  33  34  35
    36  37  40  41  42  43  44  46  47  48  49  50  52  53  54  55  56  58  59  60  61  62
    64  65  66  67  68  70  71  72  73  74  76  77  78  79  80  82  83  84  85  86
chain bonds :
    2-8   5-93  8-12  27-31  34-38  83-87
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   14-15  14-18  15-16  16-17  17-18  19-20  19-23  20-21
    21-22  22-23  26-27  26-30  27-28  28-29  29-30  33-34  33-37  34-35  35-36  36-37  40-41
    40-44  41-42  42-43  43-44  46-47  46-50  47-48  48-49  49-50  52-53  52-56  53-54  54-55
    55-56  58-59  58-62  59-60  60-61  61-62  64-65  64-68  65-66  66-67  67-68  70-71  70-74
    71-72  72-73  73-74  76-77  76-80  77-78  78-79  79-80  82-83  82-86  83-84  84-85  85-86
exact/norm bonds :
    5-93  8-12  27-31  34-38  40-41  40-44  41-42  46-47  46-50  47-48  52-53  52-56  53-54
    58-59  58-62  59-60  65-66  71-72  77-78  83-87
exact bonds :
    2-8   14-15  14-18  15-16  16-17  17-18  19-20  19-23  20-21  21-22  22-23  26-27  26-30
    27-28  28-29  29-30  33-34  33-37  34-35  35-36  36-37  42-43  43-44  48-49  49-50  54-55
    55-56  60-61  61-62  64-65  64-68  66-67  67-68  70-71  70-74  72-73  73-74  76-77  76-80
    78-79  79-80  82-83  82-86  83-84  84-85  85-86
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
    containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :


G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

Match level :
    1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  12:CLASS
    14:Atom
```

```
           15:Atom   16:Atom   17:Atom   18:Atom   19:Atom   20:Atom   21:Atom   22:Atom   23:Atom
26:Atom    27:Atom   28:Atom   29:Atom   30:Atom   31:CLASS  33:Atom   34:Atom   35:Atom   36:Atom
37:Atom    38:CLASS  40:Atom   41:Atom   42:Atom   43:Atom   44:Atom   46:Atom   47:Atom   48:Atom
49:Atom    50:Atom   52:Atom   53:Atom   54:Atom   55:Atom   56:Atom   58:Atom   59:Atom   60:Atom
61:Atom    62:Atom   64:Atom   65:Atom   66:Atom   67:Atom   68:Atom   70:Atom   71:Atom   72:Atom
73:Atom    74:Atom   76:Atom   77:Atom   78:Atom   79:Atom   80:Atom   82:Atom   83:Atom   84:Atom
85:Atom    86:Atom   87:CLASS  93:CLASS  94:CLASS
```